IOSR Journal of Environmental Science, Toxicology and Food Technology (IOSR-JESTFT)
e-ISSN: 2319-2402,p- ISSN: 2319-2399.Volume 9, Issue 5 Ver. I (May. 2015), PP 71-72
www.iosrjournals.org

2, 5-Dimethylfuran as A Bio-Fuel

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I. Introduction

Diminishing fossil fuel resources and growing concerns about global warming indicate that sustainable sources of energy are needed in the near future. Renewable biomass resources have the potential to serve as a sustainable supply of fuels and chemical intermediates. The challenge for the effective utilization of these sustainable resources is to develop cost effective production methods to transform highly functionalized carbohydrate moieties into value added chemicals. Hydroxymethylfurfural, HMF is an aldehyde and a furan compound formed during the thermal decomposition of sugars and carbohydrates. It can be produced from renewable biomass resources by the acid catalyzed dehydration of hexoses. HMF has been called a "sleeping giant" and its derivative 2,5-Dimethylfuran has been identified as a biofuel with great potential.

II. What Is DMF?

DMF is used as an octane improver for gasoline. As an alternative biofuel, DMF exhibits a number of attractive features. DMF has a 20 K higher boiling point. DMF has a high research octane number (101), which will allow for the use of high engine compression ratios for improved fuel economy. DMF is stable in storage and insoluble in water. Thus, it will not get contaminated through water absorption from the atmosphere (in comparison to the very high miscibility of ethanol). DMF consumes only one-third of the energy in the evaporation stage of its production, in comparison to that required by fermentation for ethanol. DMF is manufactured on a large-scale and low cost using cellulose (fructose or glucose).

III. Advantages Of Using Dmf As A Biofuel

i. High energy density.
ii. Insoluble in water.
iii. High octane rating.
iv. Physical properties very close to gasoline.
v. Low volatility.
vi. Stable in storage.

IV. Disadvatages

i. Toxic.
ii. Liberates Oxides of Nitrogen (NO_x) & Carbon monoxide (CO) as a product of combustion.
iii. Produces hazardous intermediates on combustion.

V. Properties

PROPERTIES	GASOLINE	ETHANOL	DMF
MOLECULAR FORMULA	C_2-C_{14}	C_2H_6O	C_6H_8O
MOLECULAR MASS (kg/mol)	100-105	46.07	96.13
DENSITY @20 °C (kg/m^3)	744.6	790.9	889.7
WATER SOLUBILITY @ 25 °C (mg/ml)	INSOLUBLE	HIGHLY SOLUBLE ≥ 100	INSOLUBLE ≤ 1.47
H/C RATIO	1.795	3.00	1.33
O/C RATIO	0.00	0.50	0.1667
GRAVIMETRIC OXYGEN CONTENT(%)	0	34.78	16.67
STOICHIOMETRIC AIR-FUEL RATIO	14.56	8.95	10.72
GRAVIMETRIC CALORIFIC VALUE (MJ/kg)	42.9	26.9	32.89
VOLUMETRIC CALORIFIC VALUE (MJ/l)	31.9	21.3	30
OCTANE RATING	96.8	107	101.3
AUTO IGNITION TEMPERATURE (°C)	257	423	285.85
LATENT HEAT OF VAPOURIZATION @ 20 °C (kJ/mol)	38.51	43.25	31.91
BOILING POINT (°C)	32.8	78.4	92
FLASH POINT (°C)	-40	13	0-1

VI. Correlation Of Dmf With Exisiting Fuels

Here is a comparision between Gasoline, Ethanol & DMF. Pure Gasoline , Ethanol & 99.8% pure DMF were used. Following are the results:

A. Energy Denisty:

DMF has a relatively high volumetric energy density (31.5 MJ/l), which is comparable to that of gasoline (32.2 MJ/l) and almost 40% higher than that of ethanol (23 MJ/l).

B. Fuel Consumption:

To provide the equivalent energy output of $1m^3$ of gasoline, 1.512 m^3 of ethanol and 1.073 m^3 of DMF were required. Of the three fuels, ethanol has the minimum volumetric calorific value. Hence, more ethanol is required to maintain the same engine load, which increases the fuel requirement and, thus, the fuel flow rate, compared to gasoline and DMF.

C. Combustion Efficiency:

Higher combustion temperature contributes to more complete combustion. Relative oxygen content in each fuel also is a vital factor which affects the level of combustion completeness. Higher the oxygen element in fuel molecule, more is the availability of oxygen during combustion that helps to increase combustion efficiency. Amongst these fuels, the oxygen content in DMF (O/C ratio = 0.1667) is lower than ethanol (O/C ratio = 0.5). Ethanol (97-97.5%) has the highest combustion efficiency followed by DMF (95.5-96%) & Gasoline (95%).

D. Thermal Efficiency:

Efficiency of DMF is similar to gasoline. Ethanol, on the other hand, has a consistently high indicated efficiency, which is probably due to its high combustion efficiency and oxygen content (35% oxygen content by mass, 18% higher than DMF). The efficiency does not drop off as suddenly as is experienced with DMF and gasoline and remains above 37%.

E. Gaseous Emission:

Gasoline and DMF share a similar trend and level of carbon monoxide (CO) emissions. Ethanol produces lower CO levels at low loads. Despite various drawbacks, ethanol produces the lowest overall emissions. The lower CO emissions of ethanol are a result of the lower combustion temperatures and suggest that the combustion is more complete. DMF has a marginally lower indicated specific CO level compared to gasoline, which further highlights the CO emissions benefit when using oxygenated biofuels. The hydrocarbon (HC) emissions for ethanol are much lower at low engine loads compared to those for DMF and gasoline; however, the difference decreases rapidly as the engine load increases. The level of total unburned HCs resulting from DMF combustion is between gasoline and ethanol because of the oxygen content; it also contains 16.67% oxygen by mass. In general, the formation of NOx is caused by high combustion temperatures.

F. **Particulate Matter Emission:** For gasoline, 62.1% of the total particles are accumulation mode particles, whereas for DMF and ethanol, this rises to 64.4 and 67.1%, respectively. DMF's lower viscosity and surface tension accounts for it.

VII. Conclusion

Compared to ethanol, DMF has an energy density higher by 60 % in volume and by 40% in mass. It consumes only one-third of the energy in the evaporation stage of its production, compared with that required to evaporate a solution of ethanol produced by fermentation for biofuel applications. The most attractive advantage is that making DMF will not compete with land and food, and therefore it can be an ideal candidate for a new generation of sustainable bio-fuel! It has very similar properties to gasoline with regards to combustion, which means that it can be easily adopted with current spark-ignition engine technologies without the need for major modifications.

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